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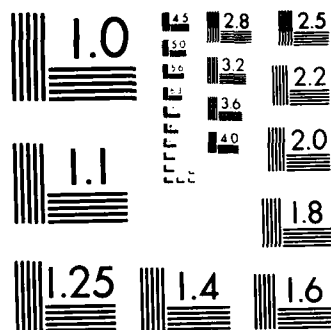
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Final Scientific Report for Contract F49620-82-C-0064,  
 "Adaptive Grid Generation Using Elliptic Generating Equations For  
 with Precise Coordinate Controls"

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 P. O. Box 8172  
 Albuquerque, N.M. 87198  
 U.S.A.

10 May 1986

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 Dr. Patrick J. Roache,  
 President and Principal Investigator

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#### A. ABSTRACT

Algorithms were developed for the generation of grids in 2D and 3D. The 3D code development involved extensive use of computer Symbolic Manipulation. A rigorous code validation procedure was developed. A controversy on the effect of strong coordinate stretching was resolved, with proof that the order of accuracy is not reduced. The contention that a well-known method always produces a non-folded grid was disproven. A family of adaptive algorithms was developed, involving both interior adaption and especially boundary adaption. Initial work was begun on an extension of the variational approach to grid generation. The grid generation algorithms have been applied in the 2D and 3D ELF codes (ELectric Field) used in the design of laser electrodes and switches. Applications are in the Pulsed Power area, including SDI research and development.

#### B. STATEMENT OF WORK

"Compatible with the level of funding, the contractor will exert his best efforts to develop numerical methods for adaptive grid generation for two- and three-dimensional internal and external flows. The numerical methods developed under the proposed contract will be documented in open-literature publications and presented at scientific and engineering meetings, and sample codes will be made available to interested users within government agencies and contractors."

#### C. STATUS OF THE RESEARCH

The algorithms and code for the generation of the 2D grid generation equations, the solution of the finite difference equations, and the verification process (see below) were all successfully developed using hand coding. The solution methods included hopscotch SOR and the much more efficient (but geometry sensitive) marching/semidirect methods.

The 3D algorithms were coded using Symbolic Manipulation methods. The work included the analytic transformation of the "hosted equations" (represented by the general second-order

equations in 3D) into general nonorthogonal coordinates, the solution of these equations by hopscotch SOR, and the coding and solution of the interior grid generation equations following Thompson et al. Symbolic Manipulation was used to perform the analytical transformations, substitute the finite difference forms, gather and simplify terms, and write a Fortran subroutine for the 3D stencil.

A rigorous validation procedure was developed for both the hosted equations and the grid generation equations. This is considered to be a major contribution of the research project. The validation procedure consists in numerically testing the truncation error convergence. An inverse procedure was devised, in which a continuum solution is specified, chosen so as to possess enough structure to exercise all the derivatives of the operator and all finite difference truncation errors. The non-homogeneous term is chosen to give the specified solution. By monitoring the truncation error as the grid is successively doubled, all aspects of the problem are verified, i.e. the transformation, the finite difference forms (validating the second order accuracy) and the iterative solution procedure. A similar procedure is followed for the grid generation equations by choosing a "solution" of a strongly twisted grid. The numerical procedure is somewhat more complicated because the solution for  $(x,y,z)$  at each point requires a nonlinear transcendental solution, performed by Newton-Raphson iteration.

These validation exercises also shed light on a controversial question regarding the effect of strong coordinate stretching on the order of accuracy of the solution of the hosted equations. All practitioners had agreed that severe inappropriate stretching would increase the size of the error, but most also were of the opinion that the order was also degraded, say from second to first order. Published analyses confirmed this, but the present work contradicted it, as did our straightforward analysis in the transformed (logical) plane. The question was settled under the present contract by performing systematic truncation error testing in 1D using extreme stretching (involving even exponentials of exponentials, requiring double precision calculations). The size of the truncation error increased greatly, as expected, but it was demonstrated that the order remained second order. The other principals involved have since revised and clarified their analysis, and the question has been settled.

The present research effort also invalidated another previous theoretical (and intuitive) result, that the Winslow method (or homogeneous Thompson-Thames-Mastin method) would always produce a non-folded grid. The present work demonstrated, by both computer solutions of practical electrode geometries and by analysis of simple problems, that the method can be made to fail in a predictable class of problems. The analysis has bearing on the well known difficulties of generating grids near airfoil trailing edges, and has been received with considerable surprise, interest and incredulity in the grid generation community.

A solution adaptive algorithm and code were developed for 2D electric field calculations. The electric field calculation typically results in a maximum electric field strength occurring on the boundary of the region, e.g. laser cavity. (This is rigorously true for the vacuum case, governed by the simple Laplacian equation.) Thus, grid adaption does not involve interior points directly but rather the location of grid points on the boundary. This aspect of grid adaption is also important in fluid dynamics but has been largely neglected. The algorithm developed here uses a first solution with boundary distribution determined by the local surface curvature. (Equidistribution in arc length is the simplest, but a weighting in surface curvature is also used.) With a first estimate of the boundary electric field values determined in this grid, a second boundary distribution is chosen to adapt to this solution. The procedure can be continued to convergence of the adapted grid, but in practice a single adapted grid is usually sufficient. The procedure was used successfully for both steady state problems, and for intra-time-step solutions of strongly nonlinear transient problems.

A family of adaptive rules was developed, with weighted combinations of equidistribution, boundary surface curvature, electric field strength (which is the gradient of the solution), curvature of the electric field, etc. (Following recommendations by Eiseman, the complete boundary surface curvature or solution curvature was used, rather than just the second derivative.) Theoretical analysis based on Taylor series and a criterion of minimizing total error indicate that, with second order accurate differencing, the grid points should be distributed so as to equidistribute the (leading terms of) the truncation error. However, the present work showed that this is impractical, since the resulting system is too stiff and overly sensitive to noise in the solution. Several other research projects have come to the same conclusion, for a variety of different systems. Also, in the present case, it was determined that a practical criterion should not even be based entirely on accuracy, but should be strongly weighted to resolution; i.e. larger error was allowed in favor of more closely resolving the maximum value of the electric field.

Although conceptually clear, the implementation of this boundary adaption involved a subtle procedure of "projective interpolation", necessitated by the fact that the continuum surface and the adapted boundary grid points do not have the same domain of definition. The problem was successfully and unambiguously resolved in 2D, but the analogous 3D problem has not been solved.

Several algorithms were also developed for the adaption of the interior grid lines. The most successful was a minor extension of the method of Thomas and Middlecoff. Unfortunately, all the algorithms tested greatly slowed the iterative convergence of the grid solution procedure. This was also true of the several algorithms developed for the interior boundary

problem, i.e. interior grid adaption with precise control of interior points at selected locations (e.g. separated shear layers or internal dielectric surfaces). The precise placement of points is straightforward, but by itself can result in discontinuities in the grid smoothness and/or coordinate line angles unless these are controlled on each side of the interior boundary. The algorithms developed here (minor extensions of the methods of Steger and Sorenson and of Thomas and Middlecoff) were only marginally successful, in that the iterative solution was slow and fragile.

Several iterative solutions methods were devised for solving the grid generation equations. The GEM spatial marching methods, previously developed by the Principal Investigator, were successfully applied in semidirect nonlinear iterations to the Thompson interior generation equations in 2D. Economies result because only one initialization of the GEM algorithm is required for the two equations for  $x$  and  $y$ . The method is quite efficient for many problems, but is fragile, failing or becoming very slow for some geometries and for strong non-homogeneous terms used for interior grid control. Also, a previously unrecognized deficiency of the marching methods was discovered, in that gradient (Neumann) boundary conditions applied along boundaries lateral to the march direction cannot be solved directly unless the grid is locally orthogonal at these boundaries. Also, an improvement in the "smoother" for multigrid algorithms for the hosted equations was developed which is more expensive of computer time for simple problems but which is not sensitive to grid orientation and aspect ratio.

Initial progress has been made on formulating an extension of the variational approach to grid generation pioneered by Brackbill and Saltzman. Symbolic Manipulation will be utilized again to handle the mathematical complexity, especially in 3D and for the non-planar surface generation.

The Symbol Manipulation work and the electric field calculations were performed on Vax computers, and much of the grid generation work was performed on a super-microcomputer based on the Motorola 68000 chip. These combined systems have proven to be very effective for this work. Several talks have been given on the experiences with these systems; interest has generally been high.

The 2D and 3D adaptive grid generation algorithms developed in this work have been applied in the ELF codes (Electric Field) developed by Ecodynamics under subcontract to Tetra Corporation for the Air Force Weapons Laboratory. These codes are under extensive use at AFWL, at Tetra Corporation, and at university contractors for the design and optimization of laser electrodes and switches. Applications are in the Pulsed Power area, including SDI research and development.

#### D. TECHNICAL JOURNAL PUBLICATIONS

"Semidirect/Marching Methods and Elliptic Grid Generation", Patrick J. Roache, in Numerical Grid Generation, Elsevier Science Publishing Co., J. F. Thompson, ed., 1982, pp. 729-737. See also Applied Mathematics and Computation, Vol. 11, 1982.

"3D Electric Field Solutions in Boundary-Fitted Coordinates", Patrick J. Roache, S. Steinberg, H. J. Happ, and W. M. Moeny, Proc. 4th IEEE Pulsed Power Conference, Albuquerque, New Mexico, 6-8 June 1983.

"Unsteady 2D Electric Field Modeling with High Accuracy on Conductor Surfaces", Patrick J. Roache, H. J. Happ, and W. M. Moeny, Proc. 4th IEEE Pulsed Power Conference, Albuquerque, New Mexico, 6-8 June 1983.

"Interactive Electric Field Calculations for Lasers", Patrick J. Roache, Stanley Steinberg, and William M. Moeny, AIAA Paper 84-1655, AIAA 17th Fluid Dynamics, Plasma Physics, and Lasers Conference, Snowmass, Colorado, 25-27 June 1984.

"Using VAXIMA to Write FORTRAN Code", Stanly Steinberg and Patrick Roache, Proc. Third MACSYMA User's Conference, Schenectady, New York, 23-25 July 1984.

"Symbolic Manipulation and Computational Fluid Dynamics", Patrick J. Roache and Stanly Steinberg, AIAA Journal, Vol. 22, Oct. 1984, pp. 1390-1394.

"Symbolic Manipulation and Computational Fluid Dynamics", Stanly Steinberg and Patrick J. Roache, Jour. of Computational Physics, Vol. 57, No. 2, Jan. 1985, pp. 251-284.

"Additional Performance Aspects of the GEM Codes", Patrick J. Roache, Numerical Heat Transfer, Vol. 8, pp. 519-535, 1985.

#### E. PROFESSIONAL PERSONNEL ASSOCIATED WITH THE RESEARCH EFFORT

Dr. Patrick J. Roache, Principal Investigator  
Dr. Stanly Steinberg  
Mr. Jose' Castillo  
Mr. Paul Sery

#### F. INTERACTIONS (COUPLING ACTIVITIES)

##### (1) PRESENTATIONS AT MEETINGS, CONFERENCES, SEMINARS

"Semidirect/Marching Methods and Elliptic Grid Generation", Patrick J. Roache, Symposium on the Numerical Generation of Curvilinear Coordinate Systems and Use in the Numerical Solution of Partial Differential Equations", April 1982, Nashville, Tenn.

"3D Electric Field solutions in Boundary-Fitted Coordinates", Patrick J. Roache, S. Steinberg, H. J. Happ, and W. M. Moeny, 4th IEEE Pulsed Power Conference, Albuquerque, New Mexico, 6-8

June 1983.

"Unsteady 2D Electric Field Modeling with High Accuracy on Conductor Surfaces", Patrick J. Roache, H. J. Happ, and W. M. Moeny, 4th IEEE Pulsed Power Conference, Albuquerque, New Mexico, 6-8 June 1983.

"Symbolic Manipulation and Computational Fluid Dynamics", Invited Paper, Patrick J. Roache and Stanly Steinberg, AIAA Computational Fluid Dynamics Conference, 13-15 July 1983, Danvers, Mass.

"Timing Studies of Super-Micro-computers", R. T. Davis and Patrick J. Roache, Open Forum II Session, AIAA Computational Fluid Dynamics Conference, 13-15 July 1983, Danvers, Mass.

"Timing Studies of Super-Micro-computers", Patrick J. Roache, SIGNUM Dinner Meeting, Albuquerque, New Mexico, 18 October 1983.

"Timing Studies of Super-Micro-Computers", Patrick J. Roache, Mechanical Engineering Seminar, University of New Mexico, 25 October 1983.

"Scientific Computing on Supermicrocomputers", Patrick J. Roache, Panel Discussion, Symposium on Personal Computers, University of New Mexico, 18 February 1984.

"Computers vs. Algorithms", Patrick J. Roache, Symposium on the Impact of Large Scale Computing on Air Force Research and Development, Air Force Weapons Laboratory, Albuquerque, New Mexico, 4-6 April 1984.

"Interactive Electric Field Calculations for Lasers", Patrick J. Roache, AIAA 17th Fluid Dynamics, Plasma Physics, and Lasers Conference, Snowmass, Colorado, 25-27 June 1984.

"Grid Generation", Patrick J. Roache, Colloquium, Dept. of Mathematics and Statistics, University of New Mexico. Sept. 1984, Albuquerque, NM.

"Computer Symbol Manipulation and Its Applications", Stanly Steinberg, Colloquium, Dept of Chemical and Nuclear Engineering, University of New Mexico, Oct. 1984, Albuquerque, NM.

"Computer Symbol Manipulation and Its Applications", Stanly Steinberg, Colloquium, Dept. of Mathematical Sciences, The University of Texas at El Paso, Oct. 1984.

"Computer Symbol Manipulation and Its Applications", Stanly Steinberg, Colloquium, Dept. of Mathematics and Statistics, University of New Mexico. Nov. 1984, Albuquerque, NM.

"Computers vs. Algorithms", Patrick J. Roache, Engineering Faculty Seminar, University of Canterbury, Christchurch, New Zealand, 5 November 1984.

"Symbolic Manipulation and Computational Fluid Dynamics", Patrick J. Roache, Engineering Faculty Seminar, University of Canterbury, Christchurch, New Zealand, 7 November 1984.

## (2) CONSULTATIVE AND ADVISORY FUNCTIONS

P. J. Roache attended the First Copper Mountain Multigrid Conference organized by Colorado State University on 5-8 April 1983.

P. J. Roache and P. Eiseman co-chaired the ASME MiniSymposium on Grid Generation held at the University of Houston on 20-22 June 1983.

P. J. Roache and S. Steinberg consulted with Dr. R. L. Rapagnani and Capt. M. Trout of the Air Force Weapons Laboratory on problems of grid generation during 1982-1984.

## G. NEW DISCOVERIES, INVENTIONS, PATENTS, SPECIFIC APPLICATIONS

No inventions or patents have resulted from this work.

The 2D and 3D adaptive grid generation algorithms developed in this work have been applied in the ELF codes (ELectric Field) developed by Ecodynamics under subcontract to Tetra Corporation for the Air Force Weapons Laboratory. These codes are under extensive use at AFWL, at Tetra Corporation, and at university contractors for the design and optimization of laser electrodes and switches. Applications are in the Pulsed Power area, including SDI research and development.

The grid generation algorithms are also under study for incorporation into a large aerodynamics code at AFWL.

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